

# ChemINDEX Database

## The Professional's Version



**Dana Roth** has a BS in Chemistry from UCLA, an MS in Chemistry from Caltech and an MLS in Library Service from UCLA. Employed at Caltech since 1965, he served as the Head of Science and Engineering Libraries from 1983-1995 and is currently the chemistry librarian. His other interests are politics and history, especially the World War II era.

**A**S JONATHAN Brecher points out in the introduction to his definitive description of ChemFinder.Com, "the internet offers a wealth of data on all topics, but chemical information provides unique challenges for searching". Thus, while traditional chemical information resources such as the Combined Chemical Dictionary, Beilstein, Gmelin, and Chemical Abstracts provide access to formally published research results and data compilations for individual chemical substances, ChemFinder.Com has uniquely addressed increasingly important, publicly available, information resources on the World Wide Web.

By way of explanation, both ChemFinder.Com and ChemINDEX are interfaces that access the same database.

ChemINDEX, however, provides greatly enhanced search, display and customization features (and without any pop-up ads). The common database has indexed nearly 80K compounds (with an additional 160K synonyms) from over 800 publicly available sites.

One of the unique features of searching with ChemINDEX is the normalization of chemical names, which largely eliminates the need to search with precise names. Searching and retrieving substance information is made much easier by stripping chemical names of spaces, parentheses and other punctuation, as well as accommodating British/American spelling differences, inverting Chemical Abstracts Index Names, and including a variety of synonyms.

### An Array of Information

While the underlying ChemINDEX database focuses on access to health and safety data, physical property data and MSDS sources are also provided. Biological macromolecules are not covered since they are well indexed (e.g., Genbank, Protein Databank). Searching with ChemFinder.Com or ChemINDEX is always a welcome adventure, as a wide variety of unusual resources, not covered in traditional databases, are quickly revealed.

With the ChemFinder.Com interface, one is limited to searching with chemical names, structural diagrams, CAS Registry Numbers, molecular formulas, molecular weights, boiling and melting points (the latter two on the structure query page). ChemINDEX, however, provides opportunities to search with a much wider variety of properties, in addition to those just

mentioned, (e.g., specific gravity/density, refraction index, vapor density, water solubility, RTECS ID, flash point, evaporation rate, vapor pressure, DOT number and EPA code).

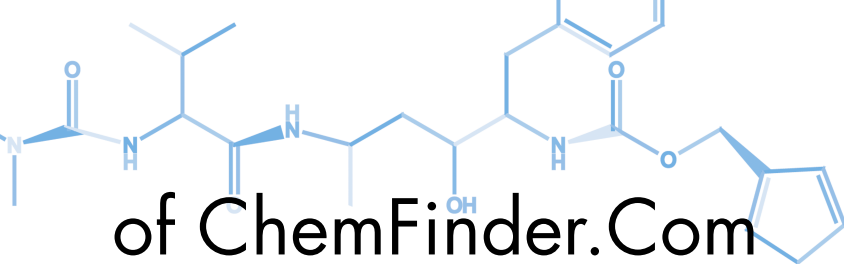
One possible problem for librarians, who provide workstations with either ChemFinder.Com or ChemINDEX for student use, is that the free ChemDraw Net Version 7.0 plug-in is user specific and ChemDraw Pro is currently required for machine specific applications. This problem will be 'corrected' with the new ChemDraw Net Version 8.0 plug-in.

Each substance record provides a property listing, including comments on color, odor, sensitivity and natural occurrence, if available. This is followed by a listing of web sites that contain additional information such as spectra. ChemFinder.Com and ChemINDEX both provide links to ChemACX Net (a supplier database), a 3-D model view, and CAS RN links both to The Merck Index (if subscribed) and to the CambridgeSoft version of the NCI Database (Cancer and AIDS screening data).

### Superior Searching

ChemINDEX clearly shows its superiority when retrieving multiple search results. Following a substructure search based on the R isomer of 2-hydroxy-3-oxo-pentane, ChemFinder.Com simply lists the chemical names for the first 25 compounds, with links to the full record. ChemINDEX, however, provides tabular data (for all 64 compounds) that also includes a structural diagram, the CAS RN and molecular formula. ChemINDEX also provides an 'edit query' button that allows one to easily return to the original search screen and change the structure or add additional search terms to refine the output.

As an aside, ChemFinder.Com and ChemINDEX may re-interpret user search statements to maximize retrieval. For example, entering C<sub>6</sub>H<sub>10</sub>O<sub>2</sub> as a search term retrieves all molecular formula



Dana L. Roth  
dzrlib@library.caltech.edu

# of ChemFinder.Com

las with C6 and H10 and O2 (including, for example, C6H10BrO2 and C6H10N2O2). Exact retrieval requires prefacing the search term with an 'equals sign' (=).

## Additional Features

Another feature of ChemINDEX is the ability to mark and export structures and associated data into ChemOffice, or other chemically enabled database programs, for the creation of private databases for personal use. In addition, ChemINDEX offers the ability to customize search and display parameters (e.g., match tetrahedral or double bond

stereo, % similarity, etc.) under the 'Preferences' menu. Marked records are saved at logoff.

## Access to NCI Database

A ChemINDEX database subscription also includes direct access to the CambridgeSoft version of the NCI database (220K compounds), which consists of the DTP (Developmental Therapeutics Program) Human Tumor Cell Line Screen and the AIDS Antiviral Screen. The ChemINDEX interface uniquely allows one to search for NCI records using structures/substructures, molecular formulas, molecular weights,

CAS RNs and synonyms. The ChemINDEX interface is a significant improvement over the standard 'government issue' NCI search screen. While not all 220K compounds have screening data, the NCI database is an excellent source of exportable structural diagrams.

## Summary

The ChemINDEX database rates a 4.9 out of 5 from this reviewer and, while I received a complimentary one year subscription for writing this review, I will soon be requesting a renewal invoice.



Frameset Page - Microsoft Internet Explorer

File Edit View Favorites Tools Help

Back Forward Stop Home Search Favorites Media Print Mail

Address http://chemindex.cambridgesoft.com/chemindex/default.asp?formgroup=basenp\_form\_group&dataaction=db&dbnbn Go Links

**ChemINDEX**  
ChemFinder.Com

Total Records 79920  
Total Hits 3

Print Preferences Help About Log Off

New Query Edit Query Refine Mark All Records Expert Hits

Record 1-3 of 3

	Structure	Name	CAS RN	Formula
Record 1 of 3 Mark Record Show Details		Breynin A		C <sub>41</sub> H <sub>58</sub> O <sub>22</sub> S
Record 2 of 3 Mark Record Show Details		Breynin B		C <sub>41</sub> H <sub>58</sub> O <sub>23</sub> S <sup>-2-2</sup>
Record 3 of 3 Mark Record Show Details		Breynolide		C <sub>15</sub> H <sub>22</sub> O <sub>7</sub> S

search entire database using entered criteria

Internet